

11.4 Maximum Entropy Analysis of the Spectroscopic Data

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It is shown how the multitude of equations usually solved within the maximum-entropy-method (MEM) scheme of the data analysis can be reduced to the number of equations equal to the number of the available experimental data. This helps to understand how the limited experimental information is distributed over much richer space of the resulting maps. Next, the MEM is shown to be an efficient tool for the analysis of the spectroscopic data with

particular emphasis on its possible use in the Mössbauer spectroscopy.

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11.5 Neutron and X-ray Scattering Study of the Magnetic Structure of ScFe₄Al₈

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The nuclear and magnetic structure refinement in the body centered tetragonal ScFe₄Al₈ single crystal is presented. The results of neutron and high resolution X-ray diffraction measurements fully confirm the nuclear order. We have studied iron magnetic ordering in the antiferromagnetic single crystal by unpolarized neutron diffraction in the temperature range 8 K - 250 K. LT neutron measurements show that the scandium compound orders with double cycloid spiral (DCS). The scandium (*2a*) site remains magnetically disordered while the iron (*8f*) site splits into two independent magnetic sublattices (orbits). Below T_{N1} ~100 K two sets of magnetic reflections were found. Each of them requires a different wave vector representation i.e. for 1st orbit (1) $\vec{q}=(0.130.130)$ and for 2nd orbit $\vec{q}_2=(0.170.170)$. Between Fe moments of adjacent chains extending along c axis (different orbits) there is a constant phase difference while along the face diagonals (the same orbit) the moments are parallel. The iron moments rotate in the plane of the wave vectors (001), but the existence of small moment component along the c-axis which would give rise to a double cone cycloid (DCC) structure and magnetic scattering contribution to the nuclear reflections cannot be excluded from the present data. The

magnetic structure seen in the single crystal studies is different from the one observed earlier by means of magnetic neutron powder diffraction [1, 2]. The reasons of this different magnetic behavior are discussed.

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11.6 Remarkable Solvent Effect on the Structure and Electrochemical Properties of [M(bipyridyl)₃](ClO₄)₃ (M = Co, Fe and Ru) Films

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In low dielectric constant media the electrooxidation of bipyridyl and phenantroline complexes of transition divalent metal cations results in the precipitation of microcrystalline film on the electrode surface. In most solvents the film is

reversibly reduced. However, films formed in the presence of acetonitrile are electrochemically inactive over a large potential range. The morphology and structure of solid phase formed on the electrode surface during the electrochemical oxidation of

bipyridyl and phenanthroline complexes of Co(II), Fe(II), and Ru(II) have been investigated by the scanning electron microscopy. The X-ray powder diffraction (XRD) measurements for bipyridyl Fe(II), Co(II) as well Co(III) complexes have been performed. A strong correlation between the electrochemical properties and the structure of the film has been found. The electrochemically inactive films of Co(II) and Fe(II) complexes formed in the presence of acetonitrile in solution consist of densely packed column-like crystallites. They exhibit monoclinic

symmetry P/2m (no. 10). The other films formed in acetonitrile free solutions, form flower-like aggregates of orthorhombic symmetry P mmm crystals (no. 47). These films are very porous.

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